(D_2CCD)

MILLIMETER-WAVE SPECTROSCOPY OF THE D_2CCD RADICAL

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The proton tunneling spectra of the D_2CCD radical has been observed by millimeter-wave spectroscopy combined with a pulsed supersonic jet expansion technique. The proton tunneling splitting ΔE_0 in the ground state was determined to be 775 MHz, which is 67% of that of H_2CCD. The barrier height of the double minimum potential 1514 cm^{-1} estimated from the ΔE_0 splitting agrees well with those for H_2CCH and H_2CCD, 1580 cm^{-1} and 1520 cm^{-1}, respectively.

α

(H/D)

0^+ 0 2

0^+ 0

(b-type) 0^+

0 (a-type)

(1)

H_2CCH[1] H_2CCD[2] $DHCCH$[3]

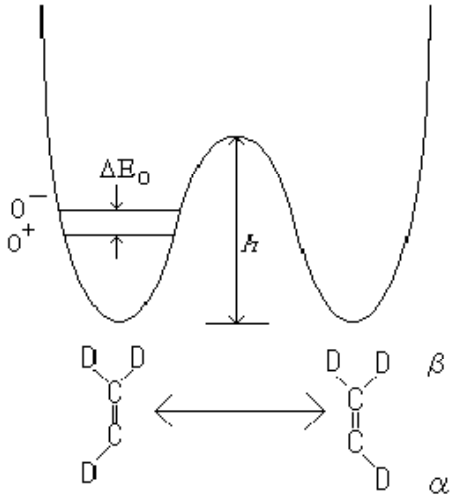

図1 対称二極小ポテンシャル

H_2CCH ΔE_0 16271.8429(59)MHz H_2CCD

1163.845(16)MHz D_2CCD FT 0^+

0 1_{01} 0_{00} (a-type) [4] 0^+ 0

(B+C)/2

A 0^+

0 (b-type) ΔE_0

A

D_2CCD D D_2CCDCl D_2CCDCl

CaC_2 D_2O C_2D_2 PCl_5 D_2O DCl

Ar H_2(3:1) D_2CCDCl 2%

8~10 20~40Hz

193nm ArF

D_2CCD

10 D_2CCD

0 ,1_{11} 0^+,0_{00}

143 500

MHz 0^+,1_{11} 0 ,0_{00}

141 950 MHz

0^+

←0 2

10

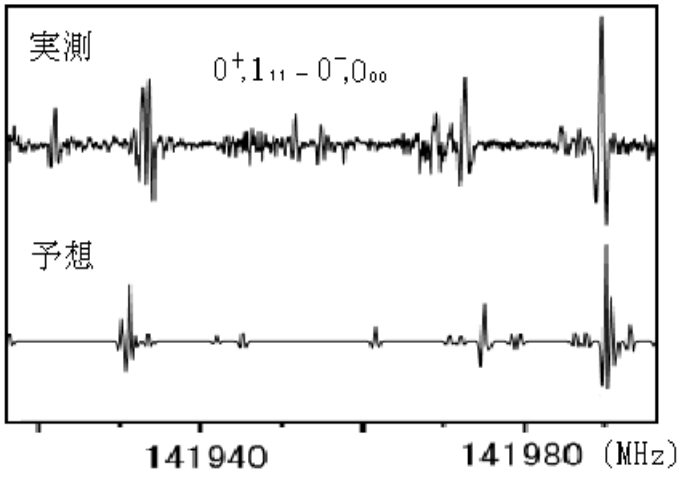

図2 トンネル回転スペクトル

3

A 122 526 MHz *ab initio* H_2CCH

D_2CCD A 122 901 MHz 0.3%

D_2CCD ΔE_0 775 MHz

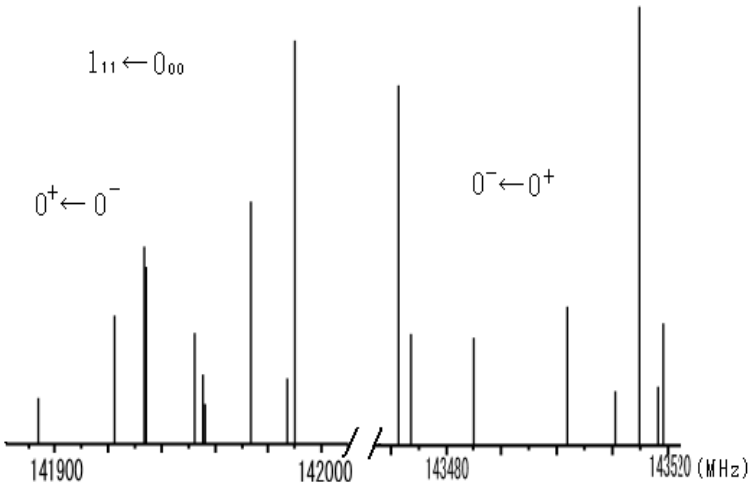

図3 観測されたトンネル回転遷移

H_2CCH 16 272 MHz H_2CCD 1165 MHz

D_2CCD

H_2CCD

67%

ΔE_0

2 –4

1

(H/D)

(h)

D_2CCD h 1514 cm^{-1} H_2CCH H_2CCD 1580cm^{-1} 1520 cm^{-1}

[1] *J. Chem. Phys.* **120**, 3604(2004) [2] (2004) p.22

[3] (2006) 3P085 [4] *J. Chem. Phys.* **116**, 10713(2002)